Crystal Structure of the Sodium Cobaltate Deuterate Superconductor $Na_xCoO_2 \cdot 4xD_2O$ ($x \approx 1/3$)

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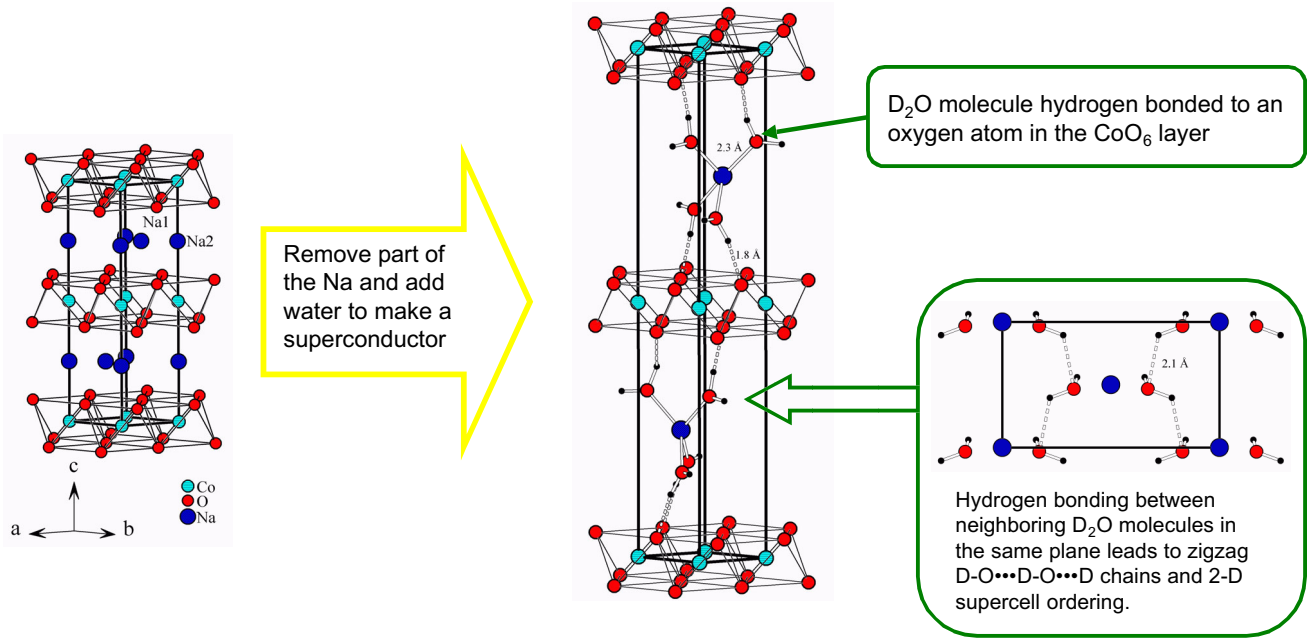
Motivation: Determine the crystal structure of the newly-discovered sodium cobaltate deuterate superconductor $Na_xCoO_2 \cdot 4xD_2O$ ($x \approx 1/3$). In particular, understand how water is incorporated and what this dictates about the chemistry of the superconducting compound.

Results:

- A single-phase deuterated sample was made by first determining the equilibrium vapor pressure for the deuterated superconducting phase.
- Neutron diffraction data were collected on the SEPD at IPNS.
- Fourier mapping revealed the general location of D_2O molecules.
- Rietveld refinement provided a detailed average structural model.
- Chemical bonding arguments led to an ordered model that explains additional scattering seen in the neutron diffraction data.



Impact: This result shows that the new superconductor is specific hydrated compound with four fully hydrogen-bonded water molecules coordinated to each Na ion, not an intercalated compound with independent and continuously variable Na and water contents or a compound with "ice" layers between the Na and CoO_6 layers. Different hydrated structures (e.g., with 6-coordinated Na) could form at other Na and water contents.

Future Work: Identify and explore the properties of other hydrated compounds in this family. Search for other layered compounds that are metallic, and superconducting, when hydrated.

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